Towards an Integrated and Efficient Framework for Leveraging Reduced Order Models for Multifidelity Uncertainty Quantification

SAND2020-0049C

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AIAA SciTech 2020
Orlando, Florida
January 6th 2020

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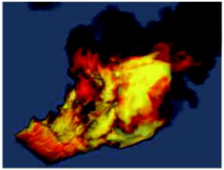
Plan of the talk

- Intro
- Multifidelity Sampling
- Reduced Order Modeling
- MF UQ-ROM coupling
- Numerical results
- Conclusions

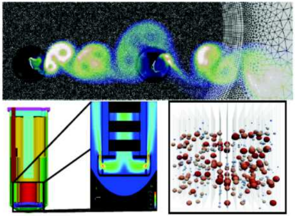
Why multifidelity in Uncertainty Quantification?

Uncertainty Quantification
DoE and DoD deployment activities

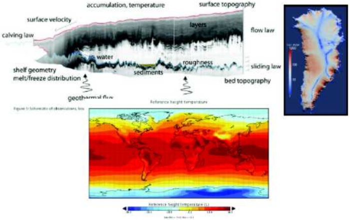
Stewardship (NNSA ASC)
Safety in abnormal environments



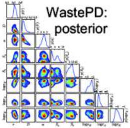
Energy (ASCR, EERE, NE)
Wind turbines, nuclear reactors

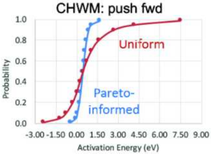


Climate (SciDAC, CSSEF, ACME)
Ice sheets, CISM, CESM, ISSM, CSDMS



Addtnl. Office of Science:
(SciDAC, EFRC)
Comp. Matls: waste forms / hazardous matls (WastePD, CHWM)
MHD: Tokamak disruption (TDS)





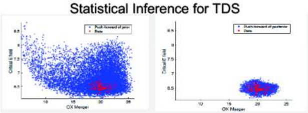


FIGURE: Courtesy of Mike Eldred

High-fidelity state-of-the-art modeling and simulations with HPC

- **Severe** simulations **budget constraints**
- **Significant dimensionality** driven by model complexity

Uncertainty Quantification for HF simulations
State-of-the-art

Two technologies are emerging as effective strategies to perform UQ for HF simulations:

- **Multifidelity** optimally fuses a handful of HF realizations with large sets of realizations from several lower fidelity models
- **Reduced Order Modeling (ROM)** creates a fast representation of the HF numerical model for a rapid *a posteriori* use

In principle ROM can be used (as it is) within a MF UQ framework as one model fidelity, however few questions need to be addressed:

- How accurate does ROM need to be to achieve a certain accuracy within the MF UQ?
- How is it possible to optimize the training step of ROM within a MF UQ workflow?

In this talk we try to explore how the coupling between ROM and MF UQ might be done efficiently

Multifidelity Sampling-based approaches

Uncertainty Quantification
Forward Propagation – Why Sampling Methods?

UQ context at a glance:

- High-dimensionality, non-linearity and possibly non-smooth responses
- Rich physics and several discretization levels/models available

Natural candidate:

- **Sampling**-based (MC-like) approaches because they are **non-intrusive**, **robust** and **flexible**...
- **Drawback:** Slow convergence $\mathcal{O}(N^{-1/2}) \rightarrow$ many realizations to build reliable statistics

Goal of the talk: **Reducing the computational cost** of obtaining MC reliable statistics

Pivotal idea:

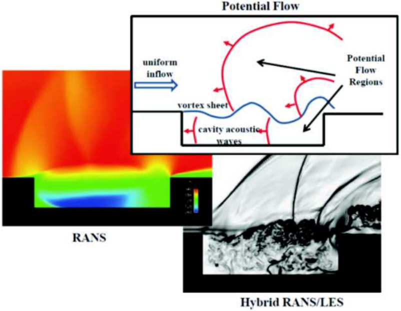
- Simplified (**low-fidelity**) models are **inaccurate** but **cheap**
  - **low-variance** estimates
- **High-fidelity** models are **costly**, but **accurate**
  - **low-bias** estimates

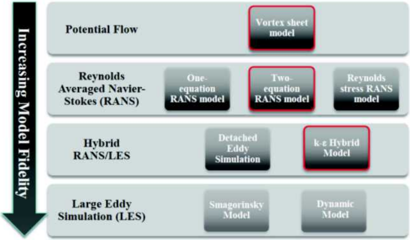
Uncertainty Quantification

Rich set of modeling choices – Discretization Vs Fidelity

Multi-fidelity: several accuracy levels available

- Physical models (Laminar/Turbulent, Reacting/non-reacting, viscous/inviscid...)
- Numerical methods (high/low order, Euler/RANS/LES, *etc*...)
- Numerical discretization (fine/coarse mesh...)
- Quality of statistics (long/short time history for turbulent flow...)





Monte Carlo simulation

Estimator variance

Problem statement: We are interested in the statistics of a functional (linear or non-linear) Q_M of the solution $\mathbf{u}_M$

$$Q_M = \mathcal{G}(\mathbf{u}_M) \quad \rightarrow \quad \mathbb{E}[Q_M]$$

- M is (related to) the number of **spatial** degrees of freedom
- $\mathbb{E}[Q_M] \xrightarrow{M \to \infty} \mathbb{E}[Q]$ for some RV $Q : \Omega \to \mathbb{R}$

$$\hat{Q}^{MC}_{M,N} \stackrel{\text{def}}{=} \frac{1}{N} \sum_{i=1}^{N} Q_M^{(i)},$$

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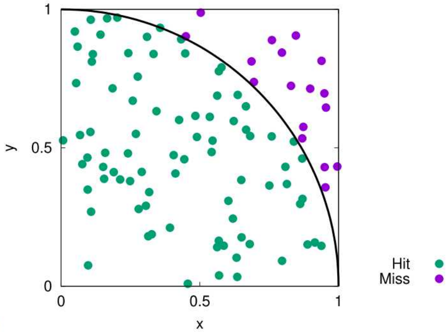
Let's use MC to compute the value $\pi \propto \frac{\#\text{Hit}}{N}$



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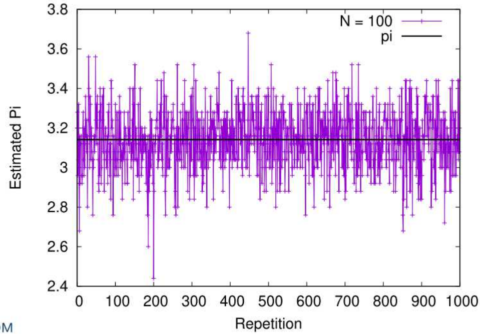

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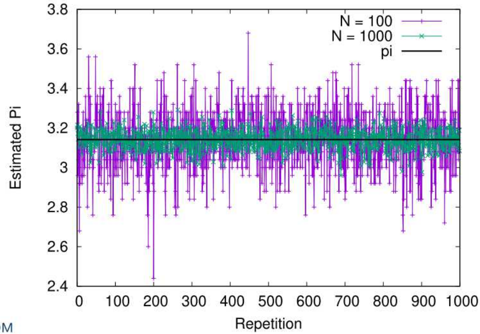


Control variate
Several ways of accelerating MC convergence

Variance of the estimator:

$$\mathbb{V}ar\left[\hat{Q}\right] = \frac{\mathbb{V}ar\left[Q\right]}{N}$$

What can we do to drive down the variance of the estimator?

#0 **Increasing the number of samples** $\rightarrow$ this is going to cost us too much for HF applications

#1 **Replace the HF model with a computational cheapest one**, *e.g.* Reduced Order Models (ROMs)

#2 Changing the QoI with another one under the assumption that its mean is the same, but the new variance is smaller (control variate)

Variance reduction techniques: sampling strategies

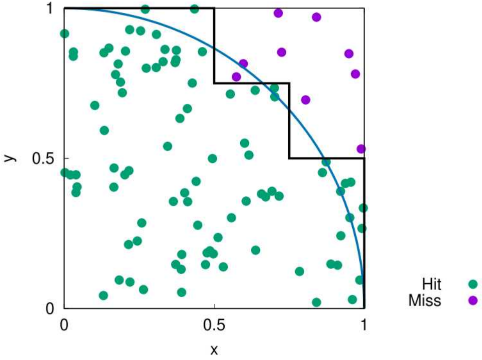
- **Importance sampling:** very useful when the main contribution to $\mathbb{E}\left[Q\right]$ comes from rare events
- **Stratified sampling:** Very effective in 1D, not always clear how to extend to multiple dimensions
- **Latin hypercube:** Effective if the function can be decomposed into a sum of 1D functions
- **(Randomized) quasi-MC:** Possibly provides better error than MC, but need to be randomized to get the confidence interval

Monte Carlo

Introducing the notion of fidelity: bias of the estimator

Numerical problems **cannot be resolved with infinite accuracy**: a discretization/numerical error is often introduced

$$\hat{Q}^{MC}_{M,N} \stackrel{\text{def}}{=} \frac{1}{N}\sum_{i=1}^{N} Q_M^{(i)}$$



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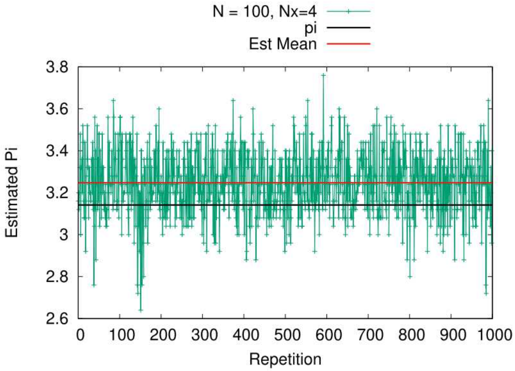

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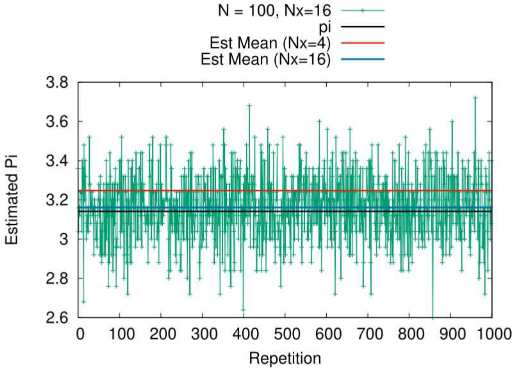

Monte Carlo simulation
Introducing the spatial discretization

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$$\hat{Q}^{MC}_{M,N} \stackrel{\text{def}}{=} \frac{1}{N} \sum_{i=1}^{N} Q_M^{(i)},$$

Looking at the **Mean Square Error (MSE)**:

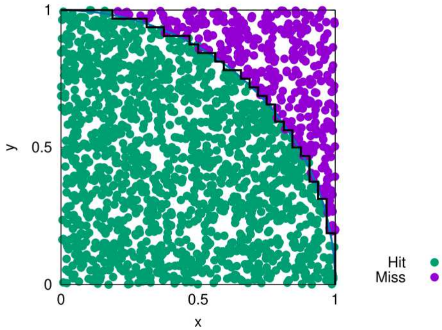
$$\mathbb{E}\left[(\hat{Q}^{MC}_{M,N} - \mathbb{E}\left[Q\right])^2 \right] = \mathbb{V}\mathbf{ar}\left[\hat{\mathbf{Q}}^{\mathbf{MC}}_{\mathbf{M,N}}\right] + (\mathbb{E}\left[\mathbf{Q_M} - \mathbf{Q}\right])^{\mathbf{2}}$$

Accelerating Monte Carlo
Bringing multiple fidelity models into the picture

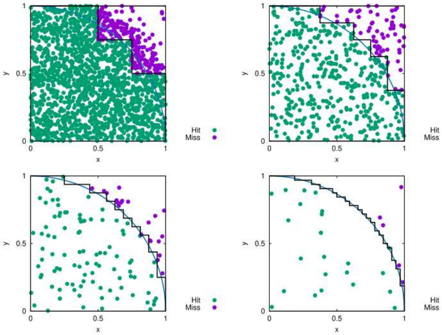
Pivotal idea:

- **High-fidelity** models are **costly**, but **accurate**
  - **low-bias** estimates
- Simplified (**low-fidelity**) models are **inaccurate** but **cheap**
  - **low-variance** estimates

Single Fidelity



Multi Fidelity



Control variate

Leveraging the correlation between models

A **Control Variate** MC estimator (function Q_1 with μ_1 **known**)

$$\hat{Q}_N^{CV} = \hat{Q} - \beta\left(\hat{Q}_1 - \mu_1\right), \quad \beta \in \mathbb{R}$$

NOTE: $\hat{Q}$ is the MC estimator of the HF and $\hat{Q}_1$ is the MC estimator of the LF

Properties:

- Unbiased, *i.e.* $\mathbb{E}\left[\hat{Q}_N^{CV}\right] = \mathbb{E}\left[\hat{Q}\right] = \mathbb{E}\left[Q\right]$ (for any β)
- $\underset{\beta}{\text{argmin}}\, \mathbb{V}ar\left[\hat{Q}_N^{CV}\right] \rightarrow \beta = -\rho \dfrac{\mathbb{V}ar^{1/2}(Q)}{\mathbb{V}ar^{1/2}(Q_1)}$
- Pearson's $\rho = \dfrac{\text{Cov}(Q, Q_1)}{\mathbb{V}ar^{1/2}(Q)\, \mathbb{V}ar^{1/2}(Q_1)}$ where $|\rho| < 1$

$$\boxed{\mathbb{V}ar\left[\hat{Q}_N^{CV}\right] = \mathbb{V}ar\left[\hat{Q}\right]\left(1 - \rho^2\right)}$$

Let's consider:

- $\mathbb{V}ar\left[Q_1\right] \approx \mathbb{V}ar\left[Q\right]$
- $\rho \approx 1$
- It follows that $\beta \approx -1$

NOTE 1: In reality β is estimated by a finite number of samples, therefore the variance is slightly higher and there is a small bias (that can be quantified)...
NOTE 2: The so-called Multilevel MC can be re-interpreted as a CV with assigned (-1) weights

Optimal Control Variate

M low-fidelity models with known expected value (In coll. with Prof. Gorodetsky, U. Michigan)

Let's consider M **low-fidelity models with known mean**. The Optimal Control Variate (OCV) is generated by adding M unbiased terms to the MC estimator

$$\hat{Q}^{\mathrm{CV}} = \hat{Q} + \sum_{i=1}^{M} \alpha_i \left(\hat{Q}_i - \mu_i \right)$$

- $\hat{Q}_i$ MC estimator for the **ith low-fidelity model**
- μ_i **known expected value** for the ith low-fidelity model
- $\underline{\alpha} = [\alpha_i, \ldots, \alpha_M]^{\mathrm{T}}$ set of **weights** (to be determined)

Let's define

- The **covariance matrix** among all the low-fidelity models: $\mathbf{C} \in \mathbb{R}^{M \times M}$
- The **vector of covariances** between the high-fidelity Q and each low-fidelity Q_i: $\mathbf{c} \in \mathbb{R}^{M}$
- $\bar{\mathbf{c}} = \mathbf{c}/\mathbb{V}ar\left[Q\right] = \left[\rho_1 \mathbb{V}ar\left[Q_1\right], \ldots, \rho_M \mathbb{V}ar\left[Q_M\right]\right]^{\mathrm{T}}$, where ρ_i is the correlation coefficient (Q, Q_i)

The optimal weights are obtained as $\underline{\alpha}^{\star} = -\mathbf{C}^{-1}\mathbf{c}$ and the variance of the OCV estimator

$$\begin{aligned} \mathbb{V}ar\left[\hat{Q}^{\mathrm{CV}}\right] &= \mathbb{V}ar\left[\hat{Q}\right] \left(1 - \bar{\mathbf{c}}^{\mathrm{T}}\mathbf{C}^{-1}\bar{\mathbf{c}}\right) \\ &= \mathbb{V}ar\left[\hat{Q}\right] (1 - R^2_{OCV}), \quad 0 \le R^2_{OCV} \le 1. \end{aligned}$$

For a single low-fidelity model: $R^2_{OCV-1} = \rho_1^2$

Approximate Control Variate

M low-fidelity models with unknown expected value (In coll. with Prof. Gorodetsky, U. Michigan)

For complex engineering models the **expected values of the M low-fidelity models are unknown** *a priori*

- Let's define the **set of sample** used for the **high-fidelity** model: $\mathbf{z}$
- Let's consider N_i **ordered evaluations** for Q_i: $\mathbf{z_i}$ (we assume $N_i = \lceil r_i N \rceil$)
- Let's partition $\mathbf{z_i}$ in two ordered subsets $\mathbf{z_i^1} \bigcup \mathbf{z_i^2} = \mathbf{z_i}$ (note that in general $\mathbf{z}_i^1 \bigcap \mathbf{z}_i^2 \neq \emptyset$)

The **generic Approximate Control Variate** is defined as

$$\tilde{Q}\left(\underline{\alpha}, \underline{\mathbf{z}}\right) = \hat{Q}(z) + \sum_{i=1}^{M} \alpha_i \left(\hat{Q}_i(\mathbf{z_i^1}) - \hat{\mu}_i(\mathbf{z_i^2}) \right) = \hat{Q}(z) + \sum_{i=1}^{M} \alpha_i \Delta_i(\mathbf{z_i}) = \hat{Q} + \underline{\alpha}^{\mathrm{T}} \underline{\Delta},$$

The **optimal weights** and **variance** can be obtained as

$$\underline{\alpha}^{\mathrm{ACV}} = -\mathbb{C}ov\left[\underline{\Delta}, \underline{\Delta}\right]^{-1} \mathbb{C}ov\left[\underline{\Delta}, \hat{Q}\right]$$

$$\mathbb{V}ar\left[\tilde{Q}\left(\underline{\alpha}^{ACV}\right)\right] = \mathbb{V}ar\left[\hat{Q}\right] \left(1 - \mathbb{C}ov\left[\underline{\Delta}, \hat{Q}\right]^{\mathrm{T}} \frac{\mathbb{C}ov\left[\underline{\Delta}, \underline{\Delta}\right]^{-1}}{\mathbb{V}ar\left[\hat{Q}\right]} \mathbb{C}ov\left[\underline{\Delta}, \hat{Q}\right]\right)$$

$$= \mathbb{V}ar\left[\hat{Q}\right] \left(1 - R^2_{\mathrm{ACV}}\right).$$

For a single low-fidelity model: $R^2_{ACV-1} = \frac{r_1 - 1}{r_1} \rho_1^2$

Approximate Control Variate

M low-fidelity models with unknown expected value (In coll. with Prof. Gorodetsky, U. Michigan)

In our Approximate CV paper we demonstrated that

- **Multilevel Monte Carlo (MLMC)** can be obtained as a particular instance of this scheme
- **Multifidelity Monte Carlo (MFMC)** can also be obtained as a particular instance of this scheme
- Both MLMC and MFMC can be defined with samples drawn in a recursive manner (which limits their ability to converge to OCV)
- For M=1, $R^2_{ACV-1} = \frac{\mathbf{r_1 - 1}}{\mathbf{r_1}} \rho^2$ and it can be shown that this result holds for both recursive and non-recursive sampling scheme

In this work we only consider the case with $M = 1$, therefore ACV-1 is indeed MFMC

[MLMC-1] Giles, M.B., Multilevel Monte Carlo path simulation. *Oper. Res.* **56**, 607-617, 2008.

[MLMC-2] Haji-Ali, A., Nobile, F., Tempone, R. Multi Index Monte Carlo: When Sparsity Meets Sampling, *Numerische Mathematik*, Vol. 132, 767–806, 2016.

[MFMC-1] Pasupathy, R., Taaffe, M., Schmeiser, B. W. & Wang, W., Control-variate estimation using estimated control means. *IIE Transactions*, **44**(5), 381–385, 2012

[MFMC-2] Ng, L.W.T. & Willcox, K. Multifidelity Approaches for Optimization Under Uncertainty. *Int. J. Numer. Meth. Engng* 100, no. 10, pp. 746772, 2014.

[MFMC-3] Peherstorfer, B., Willcox, K. & Gunzburger, M., Optimal Model Management for Multifidelity Monte Carlo Estimation. *SIAM J. Sci. Comput.* 38(5), A3163A3194, 2016.

[ACV] Gorodetsky, A., Geraci, G., Eldred, M., Jakeman, J., A Generalized Approximate Control Variate Framework for Multifidelity Uncertainty Quantification. *arXiv:1811.04988 [stat.CO]*.

Multifidelity Control Variate
Variance reduction and optimal solution

We want to solve the following problem

- Minimization of the **total computational cost**: $\mathcal{C}^{tot}\left(N^{\mathrm{HF}}, r\right) = N^{\mathrm{HF}}\mathcal{C}^{\mathrm{HF}} + rN^{\mathrm{HF}}\mathcal{C}^{\mathrm{LF}}$
- We want to reach a **target MSE** of ε^2, therefore $\mathbb{V}\mathbf{ar}\left[\hat{\mathbf{Q}}^{\mathbf{CV}}\right] = \varepsilon^2/2$

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More formally, let's define our optimization problem (Lagrange constrain optimization)

$$\underset{N^{\mathrm{HF}}, r, \lambda}{\operatorname{argmin}} (\mathcal{L}) \quad \mathcal{L} = \mathcal{C}^{tot} - \lambda\left(\frac{1}{N^{\mathrm{HF}}}\mathbb{V}ar\left[Q_M^{\mathrm{HF}}\right]\Lambda(r) - \frac{\varepsilon^2}{2}\right)$$

$$\mathcal{C}^{tot}\left(N^{\mathrm{HF}}, r\right) = N^{\mathrm{HF}}\mathcal{C}^{\mathrm{HF}} + rN^{\mathrm{HF}}\mathcal{C}^{\mathrm{LF}}$$

$$\Lambda(r) = 1 - \frac{r-1}{r}\rho_1^2.$$

The solution of the optimization problem is obtained as

$$r^{\star} = \sqrt{\frac{\mathcal{C}^{\mathrm{HF}}}{\mathcal{C}^{\mathrm{LF}}}\frac{\rho^2}{1-\rho^2}}$$

$$N^{\mathrm{HF},\star} = \frac{\mathbb{V}ar\left[Q_M^{\mathrm{HF}}\right]}{\varepsilon^2/2}\Lambda(r^{\star}).$$

Multifidelity Control Variate

How does it compare with MC?

- To reach a target variance of ε^2, MC needs

$$N_{MC} = \frac{\mathbb{V}ar\,[Q]}{\varepsilon^2}$$

- The MC total cost is therefore

$$\mathcal{C}_{MC}^{tot} = \mathcal{C}_{HF} N_{MC} = \mathcal{C}_{HF} \frac{\mathbb{V}ar\,[Q]}{\varepsilon^2}.$$

- ACV1 only needs

$$N_{\mathrm{ACV1}} = N_{MC} \left(1 - \frac{r^\star - 1}{r^\star} \rho^2\right)$$

- ACV1 total cost is

$$\mathcal{C}_{\mathrm{ACV1}}^{tot} = \mathcal{C}_{MC}^{tot} \left(1 - \frac{r^\star - 1}{r^\star} \rho^2\right) \left(1 + r^\star \frac{\mathcal{C}_{LF}}{\mathcal{C}_{HF}}\right)$$

- The ACV1 normalized cost w.r.t. MC is

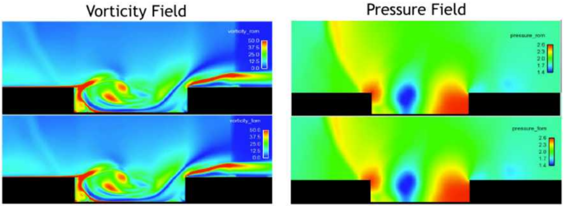
$$\mathcal{C}_{\mathrm{ACV1}}^{norm} = \left(1 - \frac{r^\star - 1}{r^\star} \rho^2\right) \left(1 + r^\star \frac{\mathcal{C}_{LF}}{\mathcal{C}_{HF}}\right).$$

Reduced Order Modeling (ROM)

Reduced order Modeling
Generalities

LSPG ROM
- 32 min, 2 cores

High-fidelity
- 5 hours, 48 cores



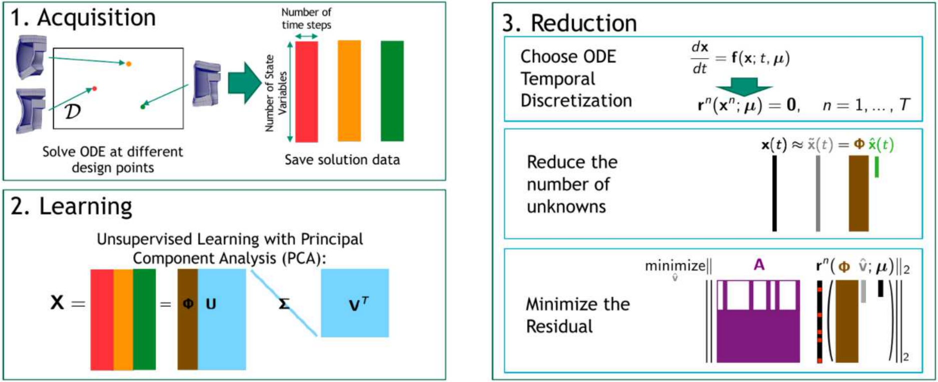
ROM are used at Sandia for
- **Time critical decision:** Model predictive control and health monitoring
- **Many queries workflows:** Optimization and Uncertainty Quantification

Model Reduction Criteria
- **Accuracy:** achieve less than 1% error
- **Low cost:** achieve at least 100x computational saving
- **Property preservation:** preserves important physical properties
- **Generalization:** should work in every difficult cases
- **Certification:** accurately quantify the ROM error
- **Extensibility:** should work for many application codes

Reduced order Modeling
Least-squares Petrov-Galerkin (LSPG) – Workflow

High-Fidelity system of ODEs:

$$\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}, t; \boldsymbol{\mu}), \qquad \boldsymbol{x}(0; \boldsymbol{\mu}) = \boldsymbol{x}^0(\boldsymbol{\mu})$$



- LSPG references: [Carlberg, Bou-Mosleh, Farhat, 2011; Carlberg, Barone, Antil, 2017]

Multifidelity UQ - ROM coupling

Multifidelity UQ and ROM coupling
Normalized cost with *a priori* ROM

- The variance reduction of the multifidelity scheme is

$$\mathbb{V}ar\left[\hat{Q}_N^{MF}\right] = \mathbb{V}ar\left[\hat{Q}\right]\left(1 - \frac{r-1}{r}\rho_1^2\right)$$

- Let's assume that ROM is the (only) LF model
- The optimal[1] number of HF and LF simulations can be obtained in closed form for an estimator variance ε^2

$$N = \frac{\mathbb{V}ar\left[Q\right]}{\varepsilon^2}\left(1 - \frac{r^\star - 1}{r^\star}\rho^2\right)$$

$$r^\star = \sqrt{\frac{\mathcal{C}_{FOM}}{\mathcal{C}_{ROM}}\frac{\rho^2}{1-\rho^2}}$$

- The overall cost of the multifidelity estimator (normalized w.r.t. MC) is

$$\mathcal{C}_{MF}^{norm} \stackrel{\text{def}}{=} \frac{\mathcal{C}_{MF}}{\mathcal{C}_{MC}} = \left(1 - \frac{r^\star - 1}{r^\star}\rho^2\right)\left(1 + r^\star\frac{\mathcal{C}_{ROM}}{\mathcal{C}_{FOM}}\right).$$

NOTES:

- The cost $\mathcal{C}_{MF}^{norm}$ represents the efficiency of the MF UQ estimator
- Given a fixed value for both $\mathcal{C}_{FOM}$ and $\mathcal{C}_{ROM}$, then $\mathcal{C}_{MF}^{norm} = \mathcal{C}_{MF}^{norm}(\rho^2)$

[1] Minimum overall estimator cost for a target estimator variance

Multifidelity UQ and ROM coupling
Online ROM's cost integration

Can we be more efficient by designing the ROM to achieve an optimal correlation and cost trade-off within this framework?

We consider here (without lack of generality) two hyper-parameters for ROM:

- n_b number of basis terms for ROM
- k the multiplicative factor that controls the time step size (*i.e.* a time step $k\Delta t$ is used for ROM whereas Δt is used for FOM)

A complexity analysis can be conducted for both FOM and ROM

- Full order model
$$\mathcal{C}^{FOM} = n_t n_{nl} n_l \nu_{nnz} N.$$
- ROM based on QR decomposition
$$\mathcal{C}^{ROM,QR} = \frac{n_t}{\mathbf{k}} n_{nl} \left(\alpha \nu_{nnz} N \mathbf{n_b} + 2\alpha N \mathbf{n_b^2} + \alpha N \mathbf{n_b} + \mathbf{n_b^2} \left(-\frac{2}{3} \mathbf{n_b^2} \right) \right)$$
- where
  - n_t is the number of time steps
  - n_{nl} is the number of iterations for the non-linear Newton-Raphson method
  - n_l is he number of iterations for the solution of the linear system
  - ν_{nnz} is the number of non-zero elements per row (*i.e.* spatial discretization stencil)
  - N is the number of spatial nodes
  - α is the hyper-reduction factor

Numerical results

Test case description

The Kuramoto-Sivashinsky equation

We consider the non-dimensionalized one-dimensional KS equation with homogeneous Dirichlet and Neumann boundary conditions,

$$\frac{\partial u}{\partial t} = -(u + \mathbf{c}) \frac{\partial u}{\partial x} - \frac{\partial^2 u}{\partial x^2} - \nu \frac{\partial^4 u}{\partial x^4}$$
$$x \in [0, L], t \in [0, \infty),$$
$$u(0,t) = u(L,t) = 0,$$
$$\left.\frac{\partial u}{\partial x}\right|_{x=0} = \left.\frac{\partial u}{\partial x}\right|_{x=L} = 0,$$
$$u(x,0) = u_0(x),$$

where L is the domain length ($L = 128$ in our tests), c is an advection parameter, and ν is the hyperviscosity parameter.

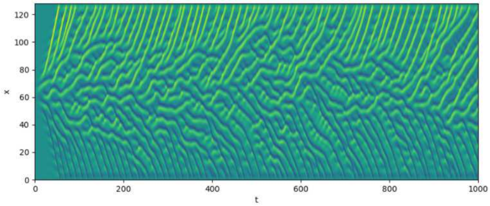


FIGURE: Space-time plot of the KS equation solution for $c = 0.0, L = 128.0, \nu = 1.0$.

Test case description
The Kuramoto-Sivashinsky equation – Quantities of Interest

In this study we considered four different quantities:

- Mean of a pointwise quantity

$$Q^1(u(x,t)) = \frac{1}{t_1 - t_0} \int_{t_0}^{t_1} u(x = 0.25L, t)\, dt,$$

- Mean of a squared pointwise quantity

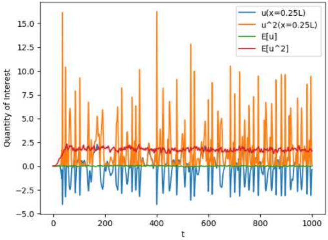
$$Q^2(u(x,t)) = \frac{1}{t_1 - t_0} \int_{t_0}^{t_1} u^2(x = 0.25L, t)\, dt,$$

- Mean of a spatially averaged quantity

$$Q^3(u(x,t)) = \frac{1}{t_1 - t_0} \int_{t_0}^{t_1} \mathbb{E}\left[u\right]\, dt, \qquad \mathbb{E}\left[u\right] = \frac{1}{L} \int_0^L u(x,t)\, dx,$$

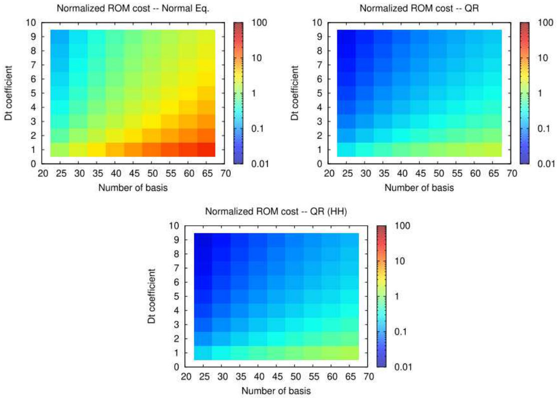
- Mean of a spatially averaged squared quantity

$$Q^4(u(x,t)) = \frac{1}{t_1 - t_0} \int_{t_0}^{t_1} \mathbb{E}\left[u^2\right]\, dt, \qquad \mathbb{E}\left[u^2\right] = \frac{1}{L} \int_0^L u^2(x,t)\, dx,$$



Test case description

Complexity analysis for FOM and ROM



- $n_t = 5000$,
- Spatial discretization stencil $\nu_{nnz} = 5$
- Grid size $N = 127$
- Linear solver iterations $n_l = 5$
- Non-linear solver iterations $n_{nl} = 15$ (FOM) and $n_{nl} = 10$ (ROM)
- Hyper-reduction factor $\alpha = 1/100$ (from literature and experience with larger problems)

MF UQ - ROM coupling

Exploring the existence of an optimal coupling region

On-line MF UQ – ROM coupling

- the hyper-parameters n_b (number of basis terms) and k (the time step factor) control the cost $\mathcal{C}_{ROM}^{norm}$
- the correlation between FOM and ROM is also a function of n_b and k
- the final MF UQ-ROM estimator's cost (normalized w.r.t. MC) is then function of n_b and k

$$\underset{n_b,k}{\text{argmin}} \left(1 - \frac{r^\star(n_b,k) - 1}{r^\star(n_b,k)} \rho^2(n_b,k)\right)\left(1 + r^\star(n_b,k)\,\frac{\mathcal{C}_{LF}^{norm}(n_b,k)}{1}\right),$$

where

$$r^\star(n_b,k) = \sqrt{\frac{1}{\mathcal{C}_{LF}^{norm}}\frac{\rho^2(n_b,k)}{1-\rho^2(n_b,k)}},$$

Numerical tests procedure:

- The uncertainty parameters are randomly sampled and the inputs for N_{train} training data points are generated;
- FOM evaluations are generated for the training data;
- A POD basis $\mathbf{\Phi}$ is computed from the aggregation of the snapshots from the N_{train} FOM evaluations;
- For an assigned value of the parameters $\bar{n}_b$ and $\bar{k}$, ROM evaluations are generated for the training data;
- The correlation and the L2 error between the FOM and ROM QoI evaluations is computed.

NOTE: the normalized L2 error is defined as follows

$$\|\mathbf{Q}_{FOM} - \mathbf{Q}_{ROM}\| = \frac{\sqrt{\sum_i \left(Q_{FOM}^{(i)} - Q_{ROM}^{(i)}\right)^2}}{\sqrt{\sum_i^{N_{train}} \left(Q_{FOM}^{(i)}\right)^2}},$$

where the vector of realizations for the FOM and ROM are denoted as $\mathbf{Q}_{FOM}$ and $\mathbf{Q}_{ROM}$, respectively.

MF UQ - ROM coupling
Numerical campaign

We performed several tests focusing on

- Understanding the impact of ROM convergence tolerance
- Understanding the differences between the predictive and reproductive cases
- Understanding the impact of the ratio between N_{train} and N_{test} for the predictive case
- Understanding the difference in performance among QoIs

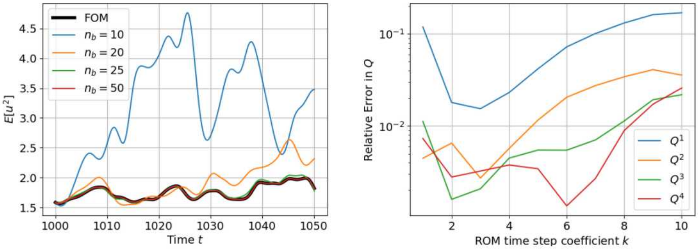
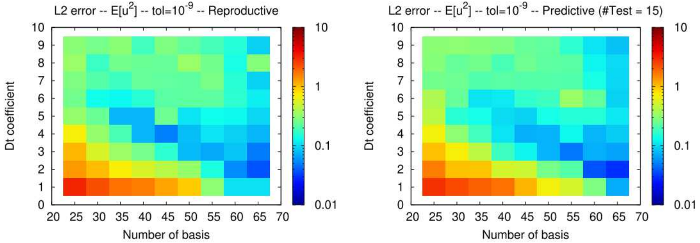


FIGURE: Time history of $\mathbb{E}\left[u^2\right]$ (left) and relative error in the quantities of interest Q^i (right).

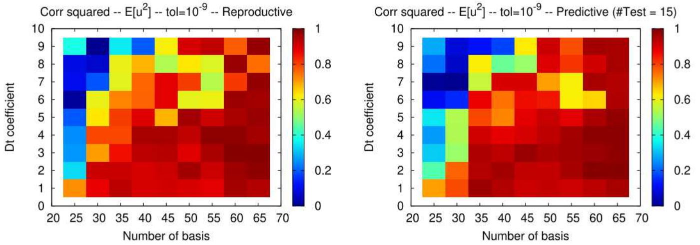
MF UQ - ROM coupling

Reproductive Vs Predictive test scenarios ($c \sim \mathcal{U}(0.1, 0.5)$ and $\nu \sim \mathcal{U}(1, 2)$)

L2 error



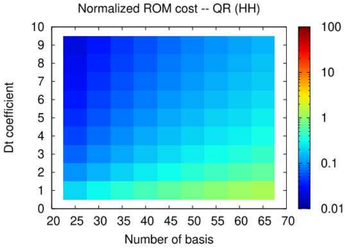
Correlation squared

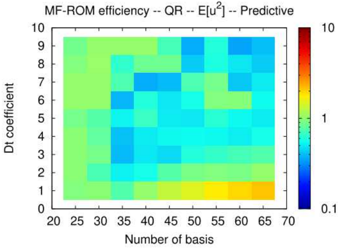


MF UQ - ROM coupling

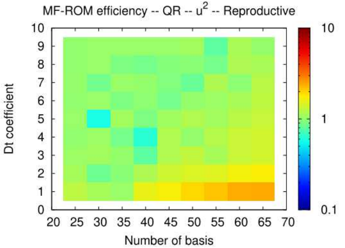
Estimator efficiency ($c \sim \mathcal{U}(0.1, 0.5)$ and $\nu \sim \mathcal{U}(1, 2)$)

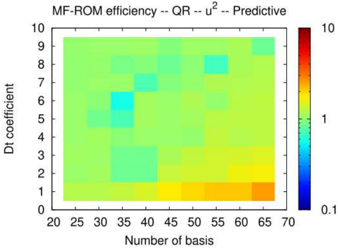
ROM (QR) – Cost and estimator efficiency for $\mathbb{E}\left[u^2\right]$





Reproductive Vs Predictive – A more challenging QoI u^2





Concluding remarks

Conclusions

Preliminary encouraging results, but more work is needed

Findings:

- A formal way of introducing and coupling ROMs with MF UQ has been developed
- In principle it is possible to tailor the ROM accuracy/cost in order to maximize the estimator efficiency (compared to a plain MC)

Challenges:

- Kuramoto-Sivashinsky is a chaotic problem which poses great challenges for all ROMs algorithms
- Integral QoIs appear easier to represent. It is difficult to achieve a good overall estimator efficiency for pointwise QoIs.
- In general, the statistics behavior is very noisy over the hyper-parameter space (might be an issue for optimization)

Future directions (work in progress):

- Explore simpler problems to improve understanding of the interplay between the deterministic accuracy and the one obtained over the stochastic space by ROMs
- Explore the cost of a truly integrated approach based on a numerical optimization of the ROM hyper-parameters

THANKS!

- Laboratory Directed Research & Development Funds @ Sandia
- Prof. Alex Gorodetsky, Univ. of Michigan
- John Jakeman, SNL

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energys National Nuclear Security Administration under contract DE-NA-0003525.

Supplemental Materials

Reduced order Modeling
Generalities

- The HF model is considered the Full Order Model from the ROM perspective
- After the semi-discretization in space a parametrized set of ODEs is obtained

$$\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}, t; \boldsymbol{\mu}), \qquad \boldsymbol{x}(0; \boldsymbol{\mu}) = \boldsymbol{x}^0(\boldsymbol{\mu}),$$

  where $\boldsymbol{x}^0(\boldsymbol{\mu})$ denotes the parameterized initial condition.
- A time-discretization method is required for the numerical solution, *e.g.* a linear k-steps method

$$\boldsymbol{r}^n(\boldsymbol{x}^n; \boldsymbol{\mu}) = \boldsymbol{0}, \quad n = 1, \ldots, N_t,$$

  where the time-discrete residual $\boldsymbol{r}^n : \mathbb{R}^N \times \mathcal{D} \to \mathbb{R}^N$ is defined as

$$\boldsymbol{r}^n : (\boldsymbol{\xi}; \boldsymbol{\nu}) \mapsto \alpha_0 \boldsymbol{\xi} - \Delta t \beta_0 \boldsymbol{f}(\boldsymbol{\xi}, t^n; \boldsymbol{\nu}) + \sum_{j=1}^{k} \alpha_j \boldsymbol{x}^{n-j} - \Delta t \sum_{j=1}^{k} \beta_j \boldsymbol{f}(\boldsymbol{x}^{n-j}, t^{n-j}; \boldsymbol{\nu}).$$

  Here, $\Delta t \in \mathbb{R}_+$ denotes the time step, $\boldsymbol{x}^k$ denotes the numerical approximation to $\boldsymbol{x}(k\Delta t; \boldsymbol{\mu})$, and the coefficients α_j and $\beta_j, j = 0, \ldots, k$ with $\sum_{j=0}^{k} \alpha_j = 0$ define a particular linear multistep scheme.

In this talk we focus on Least-Square Petrov-Galerkin

Reduced order Modeling
Least-squares Petrov-Galerkin (LSPG)

- Projection-based ROM compute an approximation $\tilde{\boldsymbol{x}} \approx \boldsymbol{x}$ that lies in a low-dimensional affine trial subspace $\tilde{\boldsymbol{x}}(t;\boldsymbol{\mu}) \in \boldsymbol{x}^0(\boldsymbol{\mu}) + \text{Ran}(\boldsymbol{\Phi})$, i.e.,

$$\tilde{\boldsymbol{x}}(t;\boldsymbol{\mu}) = \boldsymbol{x}^0(\boldsymbol{\mu}) + \boldsymbol{\Phi}\hat{\boldsymbol{x}}(t;\boldsymbol{\mu}),$$

  where $\boldsymbol{\Phi} \in \mathbb{R}^{N \times p}$ is the reduced-basis matrix of dimension $p \leq N$ ($\boldsymbol{\Phi}^T\boldsymbol{\Phi} = \boldsymbol{I}$)
- $\hat{\boldsymbol{x}} : [0,T] \times \mathcal{D} \to \mathbb{R}^p$ denotes the generalized coordinates
- $\text{Ran}(\boldsymbol{A})$ denotes the range of a matrix $\boldsymbol{A}$
- LSPG substitute the approximation $\boldsymbol{x} \leftarrow \tilde{\boldsymbol{x}}$ into the FOM ODE, and subsequently minimizes the ODE residual in a weighted ℓ^2-norm, i.e.,

$$\hat{\boldsymbol{x}}^n = \underset{\hat{\boldsymbol{z}} \in \mathbb{R}^p}{\arg\min} \|\boldsymbol{A}\boldsymbol{r}^n(\boldsymbol{x}^0(\boldsymbol{\mu}) + \boldsymbol{\Phi}\hat{\boldsymbol{z}};\boldsymbol{\mu})\|_2.$$

- To ensure an N-independent operation count a sparse weighting matrix should be selected

$$\boldsymbol{A} = (\boldsymbol{P}_r\boldsymbol{\Phi}_r)^+\boldsymbol{P}_r \quad \text{and}$$
$$\boldsymbol{A} = \boldsymbol{P}_r$$

  in the case of gappy POD and collocation, respectively.